Amendments to the Claims

This listing of claims replaces all prior versions, and listings, of claims in the above-identified application:

1. **(Original)** A molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Figure 4.

2. **(Original)** The molecule or molecular complex of claim 1, wherein the FAD binding pocket comprises the amino acids listed in Table 2.

3. **(Original)** The molecule or molecular complex of claim 1, wherein the FAD binding pocket comprises the amino acids listed in Table 3.

4. **(Original)** A molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket, wherein the substrate binding pocket comprises amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Figure 4.

5. **(Original)** The molecule or molecular complex of claim 4, wherein the substrate binding pocket comprises the amino acids listed in Table 5.

6. **(Original)** The molecule or molecular complex of claim 4, wherein the substrate binding pocket comprises the amino acids listed in Table 6.

7. **(Original)** A molecule or molecular complex that is structurally homologous to an *S. aureus* MurB molecule or molecular complex, wherein the *S. aureus* MurB molecule or molecular complex is represented by at least a portion of the structure coordinates listed in Figure 4.

8-20. **Canceled**

21. **(Withdrawn)** A method for obtaining structural information about a molecule or a molecular complex of unknown structure comprising:

crystallizing the molecule or molecular complex;

generating an x-ray diffraction pattern from the crystallized molecule or molecular complex;

applying at least a portion of the structure coordinates set forth Figure 4 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

22. **(Withdrawn)** A method for homology modeling an *S. aureus* MurB homolog comprising:

aligning the amino acid sequence of an *S. aureus* MurB homolog with an amino acid sequence of *S. aureus* MurB and incorporating the sequence of the *S. aureus* MurB homolog into a model of *S. aureus* MurB derived from structure coordinates set forth in Figure 4 to yield a preliminary model of the *S. aureus* MurB homolog;

subjecting the preliminary model to energy minimization to yield an energy minimized model;

remodeling regions of the energy minimized model where stereochemistry restraints are violated to yield a final model of the *S. aureus* MurB homolog.

23. **(Withdrawn)** A computer-assisted method for identifying an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, the FAD binding pocket comprising the amino acids listed in Table 1;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

24. **(Withdrawn)** A computer-assisted method for identifying an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 4;

supplying the computer modeling application with a set of structure coordinates of a chemical entity; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

25. **(Withdrawn)** The method of claim 23, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

26. **(Withdrawn)** The method of claim 24, wherein the substrate binding pocket comprises the amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

27. **(Withdrawn)** The method of claim 23 or 24, wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between, or the interference with, the chemical entity and the binding pocket.

28. **(Withdrawn)** The method of claim 23 or 24 further comprising screening a library of chemical entities.

29. **(Withdrawn)** A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, the FAD binding pocket comprising the amino acids listed in Table 1;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the FAD binding pocket of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

30. **(Withdrawn)** A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like substrate binding pocket, the substrate binding pocket comprising the amino acids listed in Table 4;

supplying the computer modeling application with a set of structure coordinates for a chemical entity;

evaluating the potential binding or interfering interactions between the chemical entity and the substrate binding pocket of the molecule or molecular complex;

structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and

determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

31. **(Withdrawn)** The method of claim 29, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

32. **(Withdrawn)** The method of claim 30, wherein the substrate binding pocket comprises the amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the

backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

33. **(Withdrawn)** The method of claim 29 or 30, wherein determining whether the modified chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding pocket.

34. **(Withdrawn)** The method of claim 29 or 30, wherein the set of structure coordinates for the chemical entity is obtained from a chemical fragment library

35. **(Withdrawn)** A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of an *S. aureus* MurB or MurB-like FAD binding pocket, wherein the FAD binding pocket comprises the amino acids listed in Table 1;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

36. **(Withdrawn)** A computer-assisted method for designing an inhibitor of *S. aureus* MurB activity *de novo* comprising:

supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a

portion of an *S. aureus* MurB substrate binding pocket, wherein the substrate binding pocket comprises the amino acids listed in Table 4;

computationally building a chemical entity represented by set of structure coordinates; and

determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

37. **(Withdrawn)** The method of claim 35, wherein the FAD binding pocket comprises the amino acids listed in Table 1, the FAD binding pocket being defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

38. **(Withdrawn)** The method of claim 36, wherein the substrate binding pocket comprises the amino acids listed in Table 4, the substrate binding pocket being defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

39. **(Withdrawn)** The method of claim 35 or 36, wherein determining whether the chemical entity is an inhibitor expected to bind to or interfere with the molecule or molecular complex comprises performing a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between or interference with the chemical entity and the binding pocket.

40. **(Withdrawn)** The method of any of claims 23, 24, 29, 30, 35, or 36 further comprising supplying or synthesizing the potential inhibitor, then assaying the potential inhibitor to determine whether it inhibits *S. aureus* MurB activity.

41. **(Withdrawn)** A method for making an inhibitor of *S. aureus* MurB activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* MurB activity, the chemical entity having been identified during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* MurB or MurB-like FAD binding pocket or substrate binding pocket; supplying the computer modeling application with a set of structure coordinates of a chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

42. **(Withdrawn)** A method for making an inhibitor of *S. aureus* MurB activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S. aureus* MurB activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* MurB or MurB-like FAD binding pocket or substrate binding pocket; supplying the computer modeling application with a set of structure coordinates for a chemical entity; evaluating the potential binding interactions between the chemical entity and a binding pocket of the molecule or molecular complex; structurally modifying the chemical entity to yield a set of structure coordinates for a modified chemical entity; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at the binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

43. **(Withdrawn)** A method for making an inhibitor of *S. aureus* MurB activity, the method comprising chemically or enzymatically synthesizing a chemical entity to yield an inhibitor of *S.*

aureus MurB activity, the chemical entity having been designed during a computer-assisted process comprising supplying a computer modeling application with a set of structure coordinates of a molecule or molecular complex, the molecule or molecular complex comprising at least a portion of a *S. aureus* MurB or MurB-like FAD binding pocket or substrate binding pocket; computationally building a chemical entity represented by set of structure coordinates; and determining whether the chemical entity is expected to bind to or interfere with the molecule or molecular complex at a binding pocket, wherein binding to or interfering with the molecule or molecular complex is indicative of potential inhibition of *S. aureus* MurB activity.

44-53. **Canceled**

54. **(New)** A polypeptide consisting of a portion of *S. aureus* MurB starting at one of amino acids 37 to 42 and ending at one of amino acids 310 to 312 of *S. aureus* MurB as set forth in SEQ ID NO:1.

55. **(New)** The polypeptide of claim 54, wherein the three-dimensional configuration of the amino acids listed in Table 1, is defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

56. **(New)** The polypeptide of claim 54, wherein the three-dimensional configuration of the amino acids listed in Table 2, is defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

57. **(New)** The polypeptide of claim 54, wherein the three-dimensional configuration of the amino acids listed in Table 3, is defined by a set of points having a root mean square deviation of less than about 1.7 Å from points representing the backbone atoms of said amino acids as

represented by structure coordinates listed in Figure 4.

58. **(New)** A polypeptide consisting of a portion of *S. aureus* MurB starting at one of amino acids 42 to 155 and ending at one of amino acids 274 to 309 of *S. aureus* MurB as set forth in SEQ ID NO:1.

59. **(New)** The polypeptide of claim 58, wherein the three-dimensional configuration of the amino acids listed in Table 4, is defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

60. **(New)** The polypeptide of claim 58, wherein the three-dimensional configuration of the amino acids listed in Table 5, is defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.

61. **(New)** The polypeptide of claim 58, wherein the three-dimensional configuration of the amino acids listed in Table 6, is defined by a set of points having a root mean square deviation of less than about 1.0 Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Figure 4.